Simulation of Electronic Devices at the Classical-Quantum Transition Scale

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Projects*

- Wigner function and transfer-matrix modeling of macroscopic quantum devices in 3-D
- Quantum corrections to classical drift-diffusion and hydrodynamic models in 3-D (with Lucent Technologies, Stanford University)
- Collaborative TCAD tool development (with Stanford University)

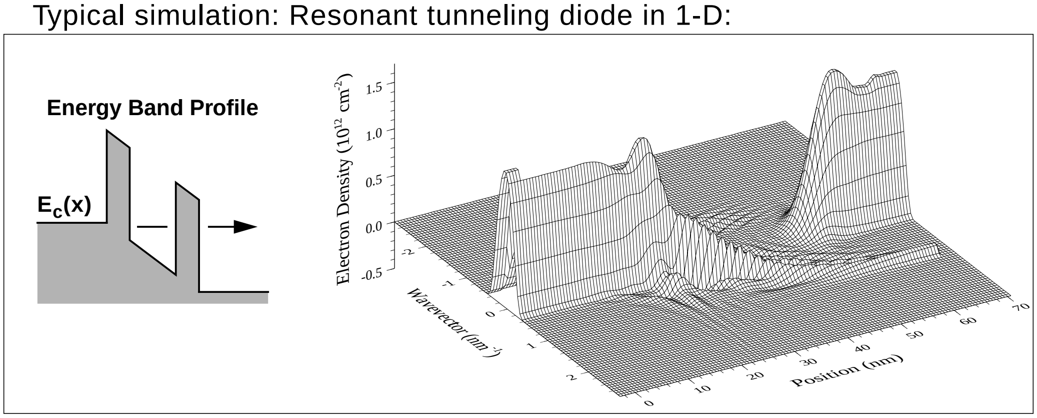
(*for details, see http://www.nas.nasa.gov/~biegel/research.html)

Quantum Device Simulation: the Wigner Function Model

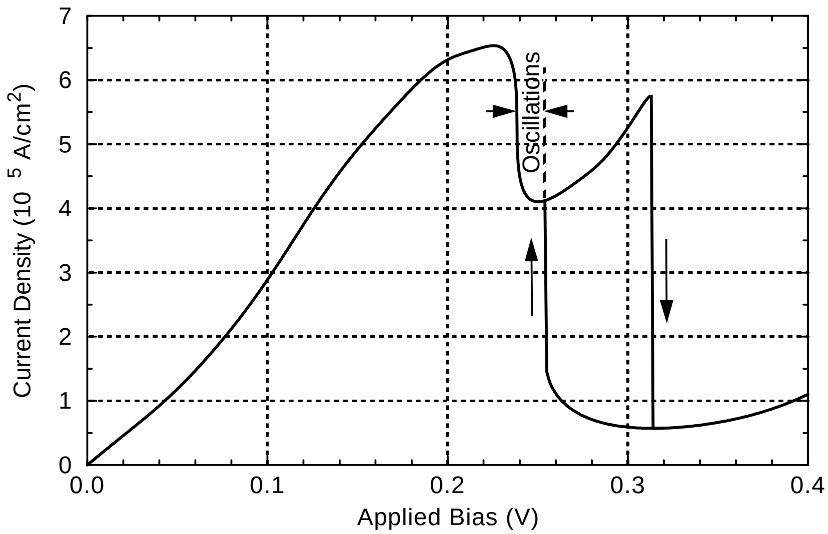
Wigner Function transport equation in 1-D:

$$\frac{\partial f_w}{\partial t} = -\underbrace{\frac{\hbar k}{m}\frac{\partial f_w}{\partial x}}_{\text{diffusion}} - \underbrace{\frac{1}{\hbar}\int\frac{dk'}{2\pi}V(x, k-k')\,f_w(x, k')}_{\text{drift}} + \underbrace{\left[\frac{\partial f_w}{\partial t}\right]_{\text{coll}}}_{\text{scatering}}$$

Typical simulation: Resonant tunneling diode in 1-D:

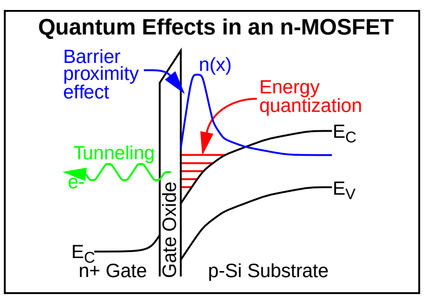


RTD Intrinsic Oscillations, Hysteresis, Bistability: Wigner Function Model Results



Plans for Wigner Function Model

- Accurate discretization of transport equation
  - consistent with other quantum models, experiment
- Computationally feasible 2-D (3-D?) simulations
- Application to quantum effects in conventional devices (MOSFET)



Quantum Corrections to Drift-Diffusion: the Density-Gradient Model

Density-Gradient Model [Ancona, *PRB* **39**(13), 9536]:

$$\nabla \cdot (\varepsilon \nabla \psi) = -q(p - n + N_D^+ - N_A^-)$$

$$\frac{\partial n}{\partial t} = \nabla \cdot [D_n \nabla n - n\mu_n \nabla(\psi + \psi_{qn})]$$

$$\frac{\partial p}{\partial t} = \nabla \cdot [D_p \nabla p + p\mu_p \nabla(\psi + \psi_{qp})]$$

Quantum potentials:

$$\psi_{qn} \equiv 2b_n\left(\frac{\nabla^2\sqrt{n}}{\sqrt{n}}\right),\ \psi_{qp} \equiv -2b_p\left(\frac{\nabla^2\sqrt{p}}{\sqrt{p}}\right),\ b_{n,\,p} \equiv \frac{\hbar^2}{12m^*_{n,\,p}q}$$

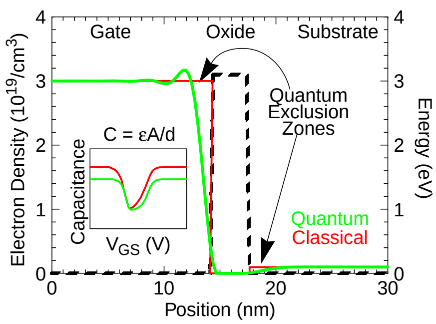
Investigative approach:

- Rapid implementation using general PDE solver (PROPHET)

Density Gradient Model Initial Results

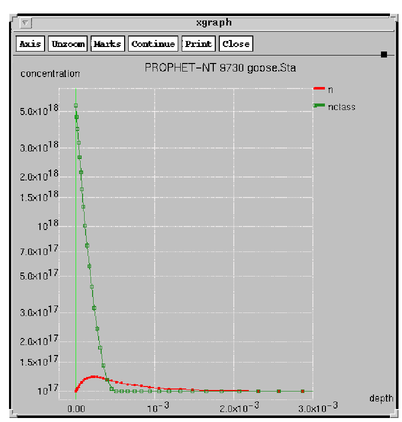
Expected Results

MOSFET with 3.3 nm Gate-Oxide:
C(x) and C-V With Quantum Correction



Electron Density Profile

(Conor Rafferty, Lucent)



Plans for Quantum Correction Models

Density-Gradient Model:

- Proof-of-concept for 1-D MOS Capacitor
- First 2-D and 3-D quantum-corrected MOSFET simulations
- Radiation effects, single-event upset phenomena
- Comparison with experimental results for ultra-small devices
- Comparison with other classical and quantum models

Quantum-Hydrodynamic Model:

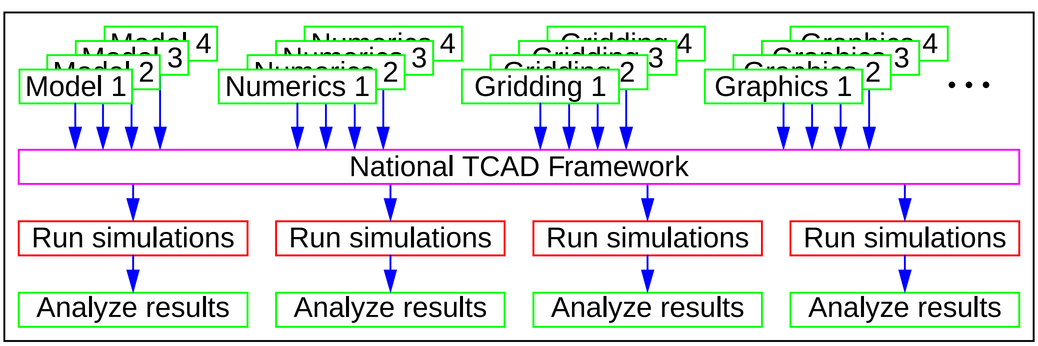
- (see above)

Answer industry's questions about quantum effects in electronic devices:

- How severe will these effects become with each device generation?
- How can these effects be suppressed?
- How can these effects be used to improve device operation?

New TCAD Development Approach: National TCAD Framework (NTF)

Modular TCAD development platform

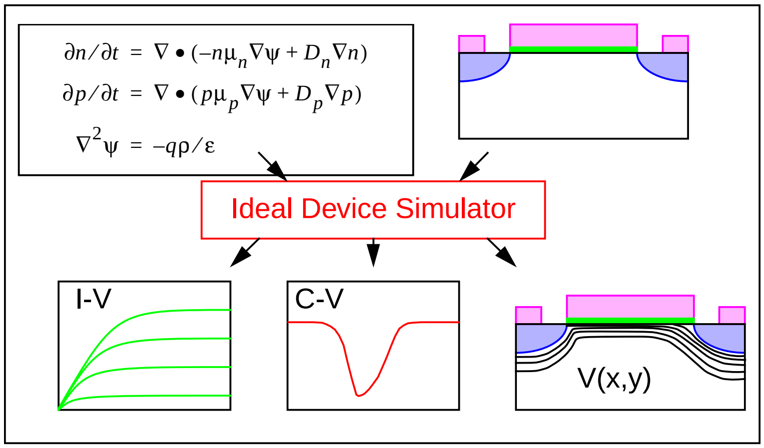


- Enables and encourages collaboration
- Well-defined functional interfaces
- Basic "glue" services

Multiply usefulness of high-level functionality

Model Developer Environment

Model specified as set of PDEs, constraints



Ideally, model independent of other code

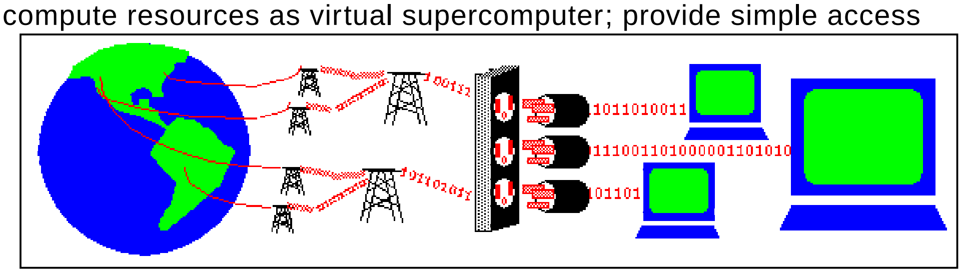
Practically, collaborate with numerical experts

Information Power Grid (IPG)

Observations:

- Many computations of interest (e.g., TCAD) beyond feasibility
- High percent of CPU cycles are wasted "bit-flips"

IPG goal: To link massive numbers of heterogeneous, distributed compute resources as virtual supercomputer; provide simple access



Principal benefits:

- transparent resource access
- load sharing/balancing
- fault tolerance, minimum loss-of-service
- economies of scale